NEUTRON TRANSPORT FROM A POINT SOURCE IN A SLAB; A COMPARISON BETWEEN DIFFUSION THEORY AND TRANSPORT THEORY

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THESIS

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September 1970

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Submitted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE IN PHYSICS

from the

NAVAL POSTGRADUATE SCHOOL
September 1970

ABSTRACT

The one-speed, steady state, diffusion equation was solved for a point source and for a normal pencil beam in a homogeneous, isotropically scattering slab. Numerical results obtained using diffusion theory were compared to available transport theory results for two slab thicknesses.

This comparison demonstrated that the diffusion theory approximation to the transport equation will yield accurate results except within about one half mean free path of a boundary and except within about three mean free paths of a source. The best agreement between diffusion theory and transport theory is obtained if the first radial buckling constant in the diffusion solution is chosen equal to the radial buckling computed using transport theory.

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I. INTRODUCTION

After being introduced into a diffusing medium, neutrons suffer numerous collisions with the atomic nuclei of the medium. The collision process is quite complicated, since either scattering, fission, or absorption can occur. As a result of streaming and repeated collisions, neutrons are constantly changing their location in the medium as well as their velocity (speed and direction). Indeed, some neutrons disappear (absorption) while others reappear (fission) while many simply change their speed and direction (scattering). The motion of any one neutron would appear to be quite random.

The statistical concept of a distribution function is convenient for describing this complicated motion. In essence, we consider "typical" neutrons and try to find the neutron density throughout a medium by using the principles of transport theory. Although these principles are straightforward and the exact equation (Boltzmann equation) governing transport phenomena can easily be derived, the solution to this equation is usually quite complicated. [1]

Only in recent years have methods been developed to obtain exact solutions to the transport equation. These methods, while yielding exact results, are highly complex and require considerable computer effort. [2] For these reasons many problems in reactor physics and shielding design have been approached using the diffusion approximation to the transport equation. However, diffusion theory is expected to yield accurate results only when the assumptions of Fick's law apply to the problem. [3]

Quite recently A. Leonard and G. Garrettson [4] developed techniques to solve the neutron transport equation exactly for the class of problems

involving multidimensional neutron sources in a one-dimensional medium. Because some numerical data was available for a certain subclass of these problems, it was felt worth-while to develop a solution to the same subclass of problems using the diffusion approximation and to compare the results with the transport solutions.

In this thesis, the Green's function for neutron diffusion in a homogeneous, isotropically-scattering slab, surrounded by a non reflecting medium, was determined using the diffusion approximation to the transport equation. In Chapter II, an analytical expression was obtained for the neutron density from a point source arbitrarily located in the slab. This was integrated to yield the neutron density from a pencil beam normally incident to the slab. A computer program was written to evaluate these expressions, and some of its features are described in Chapter III. In Chapter IV, the numerical results from transport theory are compared with those of diffusion theory.

This thesis has two objectives. First, it was hoped that by comparing the numerical results of diffusion theory with those of transport theory, accurate estimates could be made of the region in which the diffusion approximation can be expected to yield satisfactory results. Second, it was hoped a systematic method could be found to choose the parameters used in the diffusion equation to yield optimal agreement between the results of diffusion theory and transport theory.

II. THE DIFFUSION THEORY SOLUTION

A. THE EQUATION OF CONTINUITY

Under the assumptions of one-speed, steady-state, and isotropic scattering, the equation of continuity in the diffusion approximation is

$$D\nabla^2\Phi(\underline{r}) - (\Sigma_a - \nu\Sigma_f)\Phi(\underline{r}) + S(\underline{r}) = 0 \qquad 2.1$$

where D is the diffusion coefficient; $\Phi(\underline{r})$ is the one speed neutron flux as a function of position, Σ_a is the one-group absorption cross section, Σ_f is the one-group fission cross section, ν is the average number of neutrons produced per fission, and $S(\underline{r})$ represents an arbitrary source distribution function (those neutrons which have not yet suffered a collision). $S(\underline{r})$ will later be considered a point source. Under the assumptions of Fick's law, the diffusion coefficient is given by $D = \Sigma_s/3\Sigma^2$, where Σ_s is the one group scattering cross section and $\Sigma = \Sigma_a + \Sigma_f + \Sigma_s$ is the total cross section [3].

The physical interpretation of eqn. (2.1) is as follows: $-D\nabla^2\Phi(\underline{r})d^3r$ represents the leakage rate out of a volume element, d^3r, via streaming; $\Sigma_a\Phi(\underline{r})d^3r$ is the absorption rate in d^3r;$\nu\Sigma_f\Phi(\underline{r})d^3r$ is the neutron production rate in d^3r from fission; and $S(\underline{r})d^3r$ is the production rate in d^3r from any other source.

To obtain the diffusion approximation to the transport equation one must make the following assumptions (Fick's Law):

(1) The medium is infinite
(2) The medium is uniform
(3) There are no neutron sources in the medium
(4) Scattering is isotropic in the laboratory coordinate system
(5) The neutron flux is a slowly varying function of position
(6) The neutron flux is not a function of time.

The medium we consider is a homogeneous slab of thickness $\tau < \infty$ with isotropic scattering, and we solve the problem under the assumptions of one speed and steady-state. Thus assumptions (2), (4), and (6) are satisfied but (1), (3), and (5) are not.

In order to obtain the diffusion equation (2.1), it was necessary to assume the diffusing medium to be infinite in all directions [3]. However, neutrons arriving from more than a few m.f.p. (mean free paths) contribute little to the neutron current density at a given point, so the diffusion equation is expected to be reasonably valid <u>except</u> within a few m.f.p. of the boundaries.

The no source assumption, implying that all neutrons contributing to the neutron density are the result of collisions, is certainly not valid in the cases studied. The slabs we considered contained highly singular sources: the point source and the normal pencil beam source. However, since few neutrons originating from either source can be expected to survive more than a few m.f.p. without suffering a randomizing collision, diffusion theory should produce satisfactory results at distances greater than a few m.f.p. from a source.

The assumption of slowly varying flux is not satisfied near the sources or boundaries. In the derivation of Fick's Law, only first order terms in the Taylor expansion were retained [3]. Although second order terms will not contribute to the current density, terms containing third and higher order derivatives will make a contribution. Thus, it is necessary to restrict Fick's Law to regions where the second derivative of the flux does not change rapidly with distance. This specifically excludes regions near the sources we consider since both the normal pencil beam source and the point source (both represented using Dirac

delta functions) are highly singular. It should also be noted that since flux tends to vary rapidly in strongly absorbing media, it is also necessary to restrict Fick's Law to systems in which $\Sigma_a << \Sigma_s$. Such a restriction yields an average number of secondaries per collision,

$$c = \frac{\Sigma_s + \nu\Sigma_f}{\Sigma},$$

close to one [1].

From the preceding discussion, we can see that the diffusion theory approximations should produce satisfactory results in regions of the slab not too near boundaries or sources. Hopefully, our numerical results will indicate more precisely the region in which diffusion theory is accurate and the degree of inaccuracy outside this region.

B. THE BOUNDARY CONDITIONS FOR THE STEADY STATE DIFFUSION EQUATION

As is normally done in reactor boundary problems, the boundary conditions at the surface were chosen such that

$$\frac{1}{\Phi}\frac{d\Phi}{dn} = -\frac{1}{\ell} \qquad 2.2$$

where $\frac{d\Phi}{dn}$ is the normal derivative of the flux and ℓ is the extrapolation length [3]. This is equivalent to saying that the flux vanishes at a distance ℓ from the boundary. The value of ℓ was chosen such that the solution to the diffusion equation (2.1) matched as closely as possible the more rigorous solution to the transport equation within the slab (away from the boundaries where the diffusion equation is valid). For a planar free surface, transport theory shows that $\ell = 0.71\ \lambda_{tr}$ gives the best match, where λ_{tr} is the transport m.f.p. [3]. This choice of ℓ should provide good agreement between transport theory and diffusion theory in the interior of the slab. However, since the diffusion equation

is not valid near boundaries, a solution obtained by this device will not give the correct density near the boundaries (e.g., the flux does not really vanish at a distance ℓ outside the surface).

An additional boundary condition is obtained in a subcritical medium ($c < 1$). The neutron flux decreases toward zero as the distance from the source increases.

C. SOLUTION OF THE DIFFUSION EQUATION

Consider the homogeneous slab of thickness, τ, which has a total cross section, Σ, and which emits c secondaries per collision. The slab, infinite in both transverse directions, is surrounded by a vacuum or pure absorber. [See Fig. 1.] Under the assumptions of one-speed, steady state, and isotropic scattering, the equation of continuity in the diffusion approximation is given by (2.1).

Since $\Phi(\underline{r})$, the one-speed neutron flux, is a function only of the neutron density, $n(\underline{r})$, and the neutron velocity, v (assumed constant),

$$\Phi(\underline{r}) = vn(\underline{r}),$$

eqn. (2.1) can be written

$$D\nabla^2 n(\underline{r}) - (\Sigma_a - \nu\Sigma_f)n(\underline{r}) + \frac{S(\underline{r})}{v} = 0. \qquad 2.3$$

Where $x\varepsilon(\ell,\tau + \ell)$, and $y, z\ \varepsilon(-\infty,\infty)$.

It is convenient here to introduce cylindrical coordinates, $(x,\underline{\tilde{r}})$, $\underline{\tilde{r}} = (\tilde{r},\phi)$, and $\tilde{r} = \sqrt{y^2 + z^2}$, which are illustrated in Fig. 2. Since it is assumed that the external source

$$S(x,\underline{r}) \underset{r\to\infty}{\to} 0, \qquad \text{for } x\varepsilon(\ell,\tau + \ell),\ \phi\varepsilon(0,2\pi)$$

the boundary conditions for our problem are

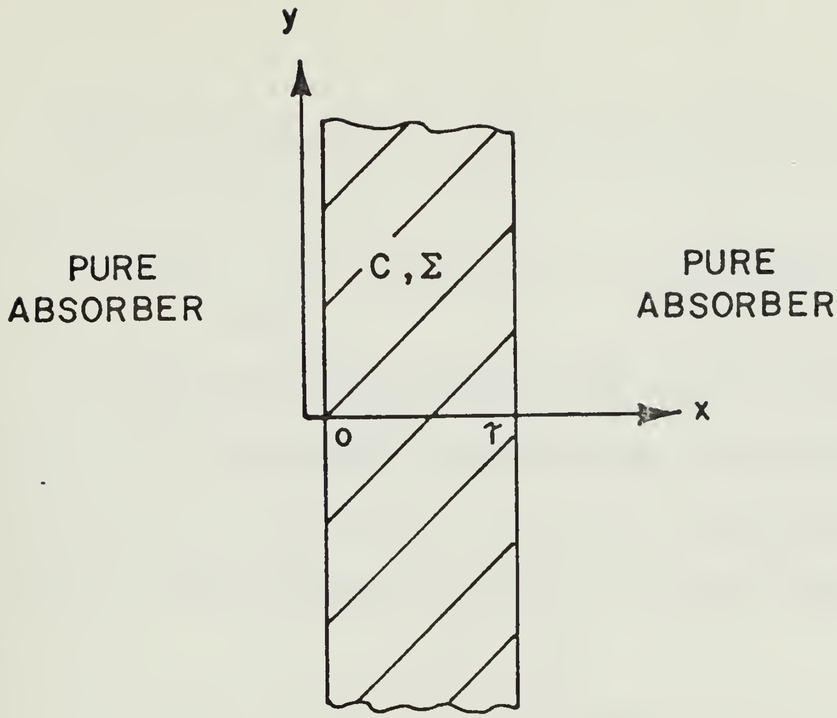

FIGURE I. A BARE HOMOGENEOUS SLAB

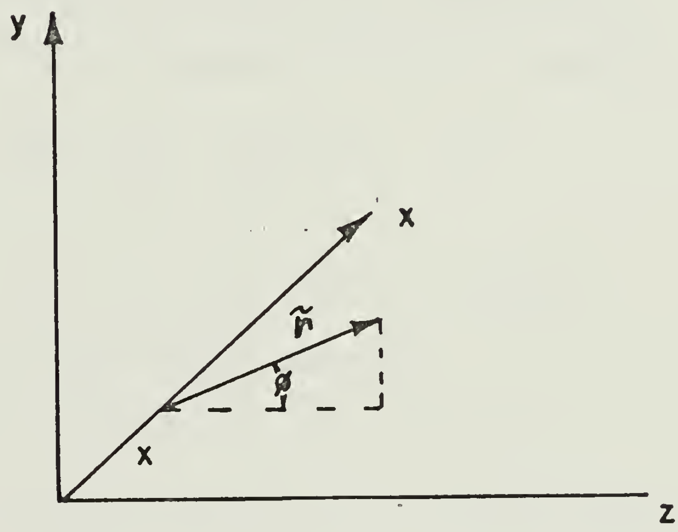

FIGURE 2. CYLINDRICAL COORDINATES

$$n(0,\underset{\sim}{r}) = n(\tau + 2\ell,\underset{\sim}{r}) = 0 \quad \text{for } \tilde{r}\ \varepsilon(0,\infty),\ \phi\varepsilon\ (0,2\pi) \qquad 2.4$$

and

$$n(x,\underset{\sim}{r}) \underset{\tilde{r}\to\infty}{\to} 0 \quad \text{for } x\ \varepsilon(\ \ell,\tau + \ell),\ \phi\ \varepsilon(0,2\pi). \qquad 2.5$$

To obtain the neutron density $n(x,\underset{\sim}{r})$ from any uncollided source, $S(x,\underset{\sim}{r})$, it is convenient to have the Green's function, $G(x,\underset{\sim}{r};\ x',\underset{\sim}{r}')$, written here as a function of cylindrical coordinates [ref. Fig. 2]. Then the formal solution to (2.3) for any source $S(\underline{r})/v$ is given by

$$n(x,\underset{\sim}{r}) = \int_0^{\tau} dx' \int_0^{2\pi} d\phi' \int_0^{\infty} d\tilde{r}'\ G(x,\underset{\sim}{r};\ x',\tilde{r}')\ \frac{S}{v}\ (x',\underset{\sim}{r}'). \qquad 2.6$$

The Green's function has the following properties:

(1) G satisfies the homogeneous differential equation

$$D\nabla^2 G - (\Sigma_a - \nu\Sigma_f)G = 0 \qquad 2.7$$

for all

$x\ \varepsilon(\ell,\tau + \ell)$, y, $z\ \varepsilon(-\infty,\infty)$, and $x \neq x'$, $\underset{\sim}{r} \neq \underset{\sim}{r}'$.

(2) G satisfies the boundary conditions

$$G(\ell,\underset{\sim}{r};\ x',\underset{\sim}{r}') = G(\tau + \ell,\underset{\sim}{r};\ x',\underset{\sim}{r}') = 0 \qquad 2.8$$

for all $x\varepsilon(\ell,\tau + \ell)$ and $y,z,y',z'\ \varepsilon(-\infty,\infty)$; [5] and $G(x,\underset{\sim}{r}'\ x',\underset{\sim}{r}') \underset{\tilde{r}\to\infty}{\to} 0.$

(3) G satisfies the proper jump condition at $\underline{r} = \underline{r}'$. In cylindrical coordinates,[9]

$$G(x,\underset{\sim}{r};\ x',\underset{\sim}{r}') \underset{\underset{\sim}{r}\to\underset{\sim}{r}'}{\longrightarrow} -\log|\underset{\sim}{r} - \underset{\sim}{r}'| \quad . \qquad 2.9$$

Equivalently, G satisfies the diffusion equation

$$D\nabla^2 G(\underline{r};\underline{r}') - (\Sigma_a - \nu\Sigma_f)G(\underline{r};\underline{r}') + \delta^3(\underline{r} - \underline{r}') = 0. \qquad 2.10$$

with a point source, $S(\underline{r}) = \delta^3(\underline{r} - \underline{r}')$, where

$\underline{r}' = (x',y',z')$, $x' \varepsilon (\ell, \tau + \ell)$, and y', $z' \varepsilon\ (-\infty,\infty)$.
$\delta^3\ (\underline{r}-r')$ is the three-dimensional Dirac delta function given by
$\delta^3(\underline{r} - \underline{r}') = \delta(x - x')\ \delta(y - y')\ \delta(z - z')$ in cartesian coordinates and
$\delta^3(\underline{r} - \underline{r}') = \delta^2(\underline{\tilde{r}} - \underline{\tilde{r}}')\ \delta(x - x')$ in cylindrical coordinates, where

$$\delta^2(\underline{\tilde{r}} - \underline{\tilde{r}}') = \frac{\delta(\tilde{r} - \tilde{r}')}{\tilde{r}}\ \delta(\phi - \phi').\ [4]$$

To solve for the Green's function one can find the eigenfunctions to the homogeneous form of equation (2.1) by separation of variables. Then $G(\underline{r};\ \underline{r}')$ can be expanded in terms of these eigenfunctions, and the expansion coefficients can be chosen so that the jump condition is satisfied [7].

In cylindrical coordinates equation (2.10) is

$$\left\{\frac{1}{\tilde{r}}\frac{\partial}{\partial\tilde{r}}\tilde{r}\frac{\partial}{\partial\tilde{r}} + \frac{1}{\tilde{r}^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial x}\right\} G(x,\underline{\tilde{r}};\ x',\underline{\tilde{r}}') - \frac{1}{D}(\Sigma_a - \nu\Sigma_f)\quad G(x,\underline{r};x',\underline{r}')$$

$$= -\frac{1}{D}\,\delta^2(\underline{\tilde{r}} - \underline{\tilde{r}}')\ \delta(x - x'). \qquad 2.11$$

Assuming a homogeneous medium and a point source located at x' on the x axis, symmetry dictates that $G(x,\underline{r};\ x',0)$ is a function of r but not of ϕ. In general then, G is a function of $|\underline{\tilde{r}} - \underline{\tilde{r}}'|$ rather than $\underline{\tilde{r}}$ and $\underline{\tilde{r}}'$ separately. Defining

$$g(x,|\underline{\tilde{r}} - \underline{\tilde{r}}'|\ ;\ x') \equiv G(x,\underline{\tilde{r}};\ x',\underline{\tilde{r}}')$$

we obtain

$$\left\{\frac{1}{\tilde{r}}\frac{\partial}{\partial \tilde{r}}\tilde{r}\frac{\partial}{\partial \tilde{r}} + \frac{\partial^2}{\partial x^2}\right\} g(x,\tilde{r};x') - Q\, g(x,\tilde{r}';x') = -\frac{1}{D}\frac{\delta^2(\tilde{r})}{\tilde{r}}\delta(x - x') \qquad 2.12$$

where we have defined the coefficient

$$Q \equiv \frac{\Sigma_a - \nu\Sigma_f}{D}. \qquad 2.13$$

$g(x,\tilde{r};x')$ satisfies the boundary conditions (2.8). For fixed $x'\varepsilon(0,\tau)$ and $\tilde{r}'(0,\infty)$, the homogeneous form of equation (2.11), satisfied by the eigenfunction $\psi(x,\tilde{r})$, is

$$\left\{\frac{\partial^2}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}}\frac{\partial}{\partial \tilde{r}} + \frac{\partial^2}{\partial x^2}\right\} \psi(x,\tilde{r}) = Q\,\psi(x,\tilde{r}). \qquad 2.14$$

To find the eigenfunction $\psi(x,r)$ we separate variables

$$\psi(x,\tilde{r}) = X(x)R(\tilde{r}),$$

and substitute into equation (2.14). This leads to the following separated eigenfunction problems:

$$\frac{d^2X}{dx^2} + L^2X = 0 \qquad 2.15$$

with boundary conditions

$$X(0) = X(\tau + 2\ell) = 0,^*$$

and

$$\frac{d^2R}{d\tilde{r}^2} + \frac{1}{\tilde{r}}\frac{dR}{d\tilde{r}} + \alpha^2 R = 0 \qquad 2.16$$

with the boundary condition

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* Note: For simplicity, the solution is forced to o at $x = 0$ and $x = \tau + 2\ell$, rather than at $\tau = -\ell$ and $x = \tau + \ell$. For numerical work and comparison with transport theory, a change of variables, $\hat{x} = x - \ell$, is introduced where $\hat{x}\ \varepsilon(0,\tau)$ is inside the slab.

$$R(r) \underset{\tilde{r}\to\infty}{\longrightarrow} 0$$

where

$$\alpha^2 \equiv Q + L^2.$$

Equation (2.15) has solutions of the form

$$X_m(x) = C_1 \sin(L_m x) + C_2 \cos(L_m x)$$

where the boundary conditions require that $C_2 = 0$ and that the eigen-values are

$$L_m = \frac{m}{\tau + 2\ell}, \quad m = 1,2,3, \cdots$$

By changing variables such that $p = \alpha_m r$, where $\alpha_m = \sqrt{Q + L_m^2}$ equation (2.16) can be reduced to the modified Bessel's equation

$$p^2 \frac{d^2R(p)}{dp^2} + p \frac{dR(p)}{dp} - p^2 R(p) = 0. \qquad 2.17$$

Since the solutions to equation (2.17) are the zeroth order modified Bessel functions $I_0(p)$ and $K_0(p)$, [6] the general solution is

$$R(p) = C_3 I_0(p) + C_4 K_0(p). \qquad 2.18$$

The boundary condition requires that $C_3 = 0$ since $I_0(p) \underset{p\to\infty}{\longrightarrow} \infty$.

Expanding the Green's function in terms of the eigenfunctions

$$X_m(x) \equiv \sin\left(\frac{m\pi x}{\tau + 2\ell}\right) \quad \text{and} \quad R_m(\tilde{r}) \equiv K_0(\alpha_m \tilde{r})$$

we obtain

$$g(x, |\underline{\tilde{r}} - \underline{\tilde{r}}'|;\ x') = \sum_{m=1}^{\infty} A_m(x')\, X_m(x)\, R_m(|\underline{\tilde{r}} - \underline{\tilde{r}}'|). \qquad 2.19$$

Since

$$X_m(x)\, R_m(\tilde{r}) = \psi_m(x, \tilde{r})$$

satisfies the homogeneous equation (2.14) and the boundary conditions (2.8), the expansion (2.19) for $G(x,\underline{r};\, x',\underline{r}')$ certainly satisfies the conditions (2.7) and (2.8) required of the Green's function. It remains only to be shown that (2.19) satisfies the jump condition (2.9). This is obtained immediately since [6]

$$K_0(\alpha_m|\underline{\tilde{r}} - \underline{\tilde{r}}'|) \underset{\underline{\tilde{r}}\to\underline{\tilde{r}}'}{\to} -\ell n\, |\underline{\tilde{r}} - \underline{\tilde{r}}'|$$

so that $R_m(r)$ satisfies the following differential equation [8]:

$$\frac{d^2R_m(\tilde{r})}{d\tilde{r}^2} + \frac{1}{\tilde{r}}\,\frac{dR_m(\tilde{r})}{d\tilde{r}} - \alpha^2_m\, R_m(\tilde{r}) = -\,\frac{2\pi\delta(\tilde{r})}{\tilde{r}} \qquad 2.20$$

Thus equation (2.19) is the proper form for the solution.

Substitution (2.19) into equation (2.10), and using the Fourier sine representation [8],

$$\delta(x - x') = \sum_{m=1}^{\infty} \frac{2}{\tau + 2\ell} \sin\left(\frac{m\pi x'}{\tau + 2\ell}\right) \sin\left(\frac{m\pi x}{\tau + 2\ell}\right), \qquad 2.21$$

as well as equation (2.20), yields

$$A_m(x') = \frac{1}{D(\tau + 2\ell)} \sin\left(\frac{m\; x'}{\tau + 2\ell}\right),$$

where we have utilized the orthogonality property

$$\int_0^{\tau+2\ell} \sin\left(\frac{m\pi x}{\tau + 2\ell}\right) \sin\left(\frac{n\pi x}{\tau + 2\ell}\right) dx = \begin{cases} 0 \text{ for } m \neq n \\ \dfrac{\tau + 2\ell}{2} \text{ for } m = n. \end{cases}$$

Therefore, recalling that $G(x,\underline{\tilde{r}};\, x',\underline{\tilde{r}}') = g(x, |\underline{\tilde{r}} - \underline{\tilde{r}}'|; x')$,

$$g(x,|\underline{\tilde{r}}-\underline{\tilde{r}}'|;x') = \sum_{m=1}^{\infty} \frac{1}{\pi D(\tau+2\ell)} \sin\left(\frac{m\pi x'}{\tau+2\ell}\right) \sin\left(\frac{m\pi x}{\tau+2\ell}\right) K_o(\alpha_m|\underline{\tilde{r}}-\underline{\tilde{r}}'|) \qquad 2.22$$

is the required Green's function for the point source problem.

It would, of course, be possible to develop the Green's function for the normal beam problems in a like manner. However, this is not necessary since equations (2.22) and (2.6) represent the formal solution to (2.3) for any source. In particular,

$$\rho(x,\tilde{r};x') = \int_0^{2\pi}\int_0^{\infty}\int_{\ell}^{\tau+\ell} g(x,|\underline{\tilde{r}}-\underline{\tilde{r}}'|;\ x')\ \ \delta^2(\underline{\tilde{r}})e^{-\Sigma x'}\ dx'\ \tilde{r}'d\tilde{r}'d\phi' \qquad 2.23$$

is the neutron density in a slab from a pencil beam normally incident to the slab at x = y = z = 0, and this function satisfies equation (2.3) with $\frac{S(\underline{r})}{v} = \delta^2(\underline{\tilde{r}})e^{-\Sigma x'}$. Thus $\rho(x,|\underline{\tilde{r}}-\underline{\tilde{r}}'|,x')$ is the Green's function for the class of problems involving neutron beams normally incident to a slab. Substitution of (2.22) into (2.23) and subsequent integration yields

$$\rho(x,\tilde{r};x') = \sum_{m=1}^{\infty} \frac{m}{D} \left\{\frac{1-(-1)^m\exp[-\Sigma(\tau+2\ell)]}{(m\pi)^2 + \Sigma(\tau+2\ell)}\right\} \sin\left(\frac{m\pi x}{\tau+2\ell}\right) K_o(\alpha_m\tilde{r}). \qquad 2.24$$

To facilitate comparison of our results with those of transport theory [1], we measure length in dimensionless units of mean free path (1 m.f.p. = $1/\Sigma$) and shift coordinates in x and x', $x \to x - \ell$, so that $x\ \varepsilon(0,\tau)$ lies inside the slab. Then the solutions (2.22) and (2.24) take the form

$$g(x,\tilde{r};x') = C \sum_{m=1}^{\infty} \sin\left(\frac{m\pi(x'+\ell)}{\tau+2\ell}\right) \sin\left(\frac{m\pi(x+\ell)}{\tau+2\ell}\right) K_o(\alpha_m\tilde{r}) \qquad 2.25$$

and

$$\rho(x,\tilde{r};x') = C' \sum_{m=1}^{\infty} \left\{ \frac{1 - (-1)^m e^{-(\tau+2\ell)}}{(m\pi)^2 + (\tau+2\ell)} \right\} \sin\left(\frac{m\pi(x+\ell)}{\tau+2\ell}\right) K_o(\alpha_m \tilde{r}), \qquad 2.26$$

where all lengths are expressed in units of mean free path. For example,

$$\alpha_m \tilde{r} = \sqrt{\frac{Q}{\Sigma^2} + \left(\frac{m\pi}{\tau\Sigma+2\ell\Sigma}\right)^2} \; (\Sigma\tilde{r}). \qquad 2.27$$

where $\Sigma\tilde{r} = \tilde{r}/(1/\Sigma)$ is the radial distance expressed in mean free paths. For equations (2.26)-(2.27), and from this point on, all distances are understood to be expressed in units of mean free path (e.g., $\Sigma(\tau+2\ell) \to \tau+2\ell$ m.f.p.). The constants C and C' will be adjusted to normalize the diffusion theory results to transport theory results at some chosen point.

III. NUMERICAL TECHNIQUES

A Fortran IV program (appendix 2) was written to compute numerical results using equations (2.25) and (2.26) for comparison with numerical data obtained by transport theory. Since both equations involve an infinite series, it was necessary to truncate the series at some point in order to obtain a solution. The purpose of this chapter is to justify the criteria used to terminate the series and also to explain the choice of the particular values used for the parameter Q/Σ^2.

A. TRUNCATION OF THE SERIES

Both equation (2.25) and (2.26) are infinite series solutions. In order to obtain numerical output, it was necessary to truncate these series at some point in the summation process. That is,

$$\sum_{m=1}^{\infty} A_m X_m(x) K_o(\alpha_m \tilde{r}) \approx \sum_{m=1}^{N-1} A_m X_m(x) K_o(\alpha_m r) \equiv S_N \qquad 3.1$$

where we choose N large enough so that R_N/S_N is less than some chosen ε, where

$$R_N \equiv \sum_{m=N}^{\infty} A_m X_m(x) K_o(\alpha_m r), \qquad 3.2$$

is the remainder term. The maximum absolute value of the $A_m X_m(x)$ terms in both equation (2.25) and (2.26) is unity. Thus the K_o Bessel function term dominates the series for $\alpha_m \tilde{r} >> 1$.

Since

$$|A_m X_m| \leq 1, \qquad R_N \leq \sum_{m=N}^{\infty} K_o(\alpha_m \tilde{r}) \qquad 3.3$$

factoring out $K_o(\alpha_N \tilde{r})$ and noting that [6]

$$K_o(p) \underset{p\to\infty}{\rightarrow} \sqrt{\frac{\pi}{2p}}\, e^{-p}, \qquad 3.4$$

with

$$\alpha_m \approx \frac{m\pi}{\tau+2\ell} \quad \text{for } m >> 1,$$

yields

$$R_N \lesssim K_o(\alpha_N\tilde{r}) \sum_{k=0}^{\infty} \sqrt{\frac{N}{k+N}} \left(e^{-\left(\frac{\pi\tilde{r}}{\tau+2\ell}\right)}\right)^k , \qquad 3.4$$

This power series can be summed to yield a convenient estimate for an upper bound of the remainder:

$$R_N \lesssim \frac{K_o(\alpha_N\tilde{r})}{1 - e^{-\left(\frac{\pi\tilde{r}}{\tau+2\ell}\right)}} . \qquad 3.5$$

In the computer program the series is truncated at N terms with N large enough so that

$$\frac{K_o(\alpha_N\tilde{r})}{S_N} < \varepsilon, \qquad 3.6$$

where we chose ε sufficiently small to give the desired accuracy. Then (3.5) yields the upper bound

$$\frac{R_N}{S_N} < \frac{\varepsilon}{1 - \exp[-\frac{\pi\tilde{r}}{t+2\ell}]} \qquad 3.7$$

for the remaining fraction. This upper bound is of the order of ε except when $\tilde{r} << \frac{\tau+2\ell}{\pi}$, so that the choice $\varepsilon = 0.0005$ should give at least three place accuracy except for small $\tilde{r}$. However, (3.7) represents a very conservative estimate of the upper bound, so we would expect good accuracy with this choice of ε even when $\tilde{r}$ is small. In fact, for $\tilde{r} = 0.05$ and N large enough so that

$$\frac{K_o(\alpha_N\tilde{r})}{S_N} < 0.0005,$$

numerical results indicate that $\frac{R_N}{S_N} < 0.001$, while (3.7) yields the conservative upper bound $\frac{R_N}{S_N} < 0.01$.

Therefore, on the basis of this discussion, it would appear that (3.6), with $\varepsilon = 0.0005$, is a sufficient truncation requirement to insure three-place accuracy.

B. CHOICE OF THE PARAMETER Q/Σ^2

In equations (2.25) - (2.27) the parameter Q/Σ^2 appears, where Q is defined in eqn. (2.13). This parameter is a function of the one group material cross section of the slab. However, the one-group cross sections depend specifically upon the energy-dependent flux, which is not available. Therefore, one would like to choose Q/Σ^2 so that diffusion theory will yield results that agree as closely as possible with the results of one-speed transport theory. In this thesis it is demonstrated how Q/Σ^2 might be chosen to accomplish this.

For comparison, this parameter was chosen in two ways. The first choice assumes diffusion theory for a medium in which there is no fission. For the second choice, it is noted that as $\tilde{r}$ increases, the transport theory solutions and the diffusion theory solutions decay like $K_o(\beta_m\tilde{r})$ and $K_o(\alpha_m\tilde{r})$, respectively, where β_m are the transport theory radial buckling modes [2]. To force diffusion theory to behave like transport theory for large $\tilde{r}$, the first buckling modes in diffusion theory and transport theory are chosen equal, $\alpha_1 = \beta_1$.

To obtain the expression for Q/Σ^2 in the first case, recall the parameters

$$Q = \frac{\Sigma_a - \nu\Sigma_f}{D} \qquad 3.8$$

and

$$c = \frac{\Sigma_s + \nu\Sigma_f}{\Sigma} \tag{3.9}$$

defined in Chapter II. In the diffusion approximation [3] $D = \Sigma_s/3\Sigma^2$, and if there is no fission ($\Sigma_f = D$). Q/Σ^2 reduces to

$$\frac{Q}{\Sigma^2} = \frac{3\Sigma_a}{\Sigma_s} = \frac{3(1-c)}{c}, \tag{3.10}$$

since $c = \Sigma_s/(\Sigma_a + \Sigma_s)$ in this case.

Recall that the diffusion approximation demands a highly scattering medium, $c \approx 1.0$, so $c = 0.9$ is chosen for the numerical work presented here. For this value of c, eqn. (3.10) yields the value $Q/\Sigma^2 = 0.333$.

For the second case the parameter Q/Σ^2 is obtained by comparing the transport theory and diffusion theory solutions. For large transverse distances from the source, $|\tilde{r}-\tilde{r}'| \gg 1$, a relatively simple transport theory solution is obtained [2] since the finite ($M < \infty$) point spectrum modes dominate the continuous spectrum modes:

$$G_{tr}(\underline{r};\underline{r}') = \sum_{m=1}^{M} \frac{K_0(\beta_m|\underline{r}-\underline{r}'|)}{\mathcal{D}_n} \Gamma_m(x)\, \Gamma_m(x') + 0\left[e^{-|\tilde{r}-\tilde{r}'|}\right] \tag{3.11}$$

where $\Gamma_m(x)$, $m = 1,2,\cdots,M$, are the transport eigenfunctions for the discrete eigenvalues $0 < \beta_1 < \beta_2 < \cdots < \beta_M \leq 1$ [2]. Using eqn. (3.4) it can be seen that the first mode dominates (3.11) for large radial arguments, $|\tilde{r}-\tilde{r}'| \gg 1$:

$$G_{tr}(\underline{r};\underline{r}') = \frac{1}{\mathcal{D}_1} K_0(\beta_1|\tilde{r}-\tilde{r}'|)\, \Gamma_1(x)\, \Gamma_1(x') + 0\left[\frac{e^{-\beta_2|\tilde{r}-\tilde{r}'|}}{|\tilde{r}-\tilde{r}|^{1/2}}\right].$$

Likewise, the first mode $m = 1$ dominates the diffusion theory solution (2.25) for $|\tilde{r}-\tilde{r}'| \gg 1$. Therefore, if we choose the first radial buckling modes to be equal, $\alpha_1 = \beta_1$, the two solutions will behave similarly for $|\tilde{r} - \tilde{r}'| \gg 1$.

With this choice for $\alpha_1 = \left[\frac{Q}{\Sigma^2} + \left(\frac{\pi}{\tau+2\ell}\right)^2\right]^{1/2}$, the following expression is obtained for Q/Σ^2:

$$\frac{Q}{\Sigma^2} = \beta_1^2 - \left(\frac{\pi}{\tau+2\ell}\right)^2 . \tag{3.12}$$

Numerically this corresponds to $Q/\Sigma^2 = 0.2757$, for $c = 0.9$ and $\tau = 10$ and to $Q/\Sigma^2 = 0.1918$, for $c = 0.9$ and $\tau = 3$. [2]

IV. DISCUSSION OF RESULTS AND CONCLUSIONS

The following results were obtained using the computer program discussed in Chapter III. The cases presented are those for which the exact solution has been obtained by G. Garrettson [2] using transport theory. The purpose of this chapter is to compare the results obtained using diffusion theory with those obtained using transport theory and to evaluate the performance of diffusion theory for problems of this class. These comparisons were done for cases of homogeneous slabs of thickness $\tau = 10$ and $\tau = 3$ m.f.p. (mean free paths) surrounded by a non-reflecting medium, under the assumption of one speed, steady state, and isotropic scattering. All graphical results (Figs. 3 to 17) discussed in this chapter are found in Appendix 1.

The first results presented, Figs. 3-6, are those for a pencil beam, normally incident at (0,0,0) to a slab of thickness $\tau = 10$ m.f.p., with a multiplication constant $c = 0.9$. The data has been normalized to the transport theory results at $\check{r} = 4.4448$, $x = 5.1282$ in order to facilitate the comparison. Figures 7-10 depict the results obtained from a pencil beam normally incident at (0,0,0) to a slab of thickness $\tau = 3$ m.f.p. with $c = 0.9$. Figures 7 and 8 were normalized at $\tilde{r} = 2.01$, $x = 1.5$, while Figs. 9 and 10 were normalized at $\tilde{r} = 0.2$, $x = 1.5$. Finally, Figs. 11-16 represent a comparison of the point source solutions in a slab of thickness $\tau = 10$, with $c = 0.9$, for point sources located at depths of 1 and then 5 m.f.p.

In all but Figs. 11-13 the diffusion solutions are presented for both values of Q/Σ^2 discussed in Chapter III. In this chapter, and in Appendix 1, Q/Σ^2 is referred to simply as Q, since $\Sigma = 1$ in units of mean free path.

A. COMPARISON OF NORMAL BEAM SOLUTIONS

It is interesting to note the evolution of the neutron density from a pencil beam, $N(x,\tilde{r})$, vs. $x \in [0,\tau]$, as the radial distance, $\tilde{r}$, increases. For very small $\tilde{r}$ (ref. Figs. 3, 9, and 10), the neutron density tends to have the same shape as the once-collided neutron density, which in turn resembles the uncollided density (a step function times an exponential). Transport theory predicts a very sharp discontinuity near the boundaries which is physically explained by the surface leakage [2]. Although diffusion theory correctly yields an exponentially decaying density within the slab,* it does not yield the steep gradient given by transport theory within about one half m.f.p. of either surface. The results of the two theories diverge partly because transport theory accounts for the preferential streaming toward the boundaries while diffusion theory does not. In fact, as previously discussed, the diffusion equation is simply not valid near boundaries. (Ref. Chapter II).

For any $x \in (0,\tau)$, the diffusion theory solution appears to be most inaccurate for small radial distances, $\tilde{r} < 1$. This inaccuracy is apparent from both the normal beam and point source data (ref. Figs. 3, 9, 10, 11, and 14), and it arises partly because diffusion theory does not consider the preferential streaming from a singular source in the region of the source. Since Fick's Law is derived under the assumption that there are no sources in the medium (ref. Chapter II) we should not expect the diffusion results to be accurate near sources. In fact, within one m.f.p. of the source, the errors induced by using diffusion theory may be as large as 80 percent. However, beyond about three m.f.p. the two theories yield nearly identical results (if Q is computed using eqn. (3.12)).

---

* Recall that a straight line on a semilog plot corresponds to an exponential.

B. COMPARISON OF POINT SOURCE SOLUTIONS

For solutions to the point source problem, the most noticeable discrepancy between the transport and diffusion data appears in the region within about one m.f.p. of the source (ref. Figs. 11 and 14). As previously mentioned, diffusion theory's inaccuracy near sources is partially due to its failure to consider the preferential streaming in the region of the source. As the distance from the source is increased, the relative error decreases unless a boundary region is encountered. As expected, within one half m.f.p. of the boundary, the diffusion theory solution begins to diverge until a discrepancy of about 20 percent is noted at the edges.

C. CHOICE OF THE PARAMETER Q

It should be noted (ref. Figs. 5, 7, 8, and 16) that for large radial distances, $\tilde{r}$, the agreement between transport and diffusion theory can be greatly enhanced by the proper choice of the parameter Q (ref. Chapter III). The diffusion theory yields $Q = \frac{3(1-c)}{c}$ for a medium in which there is no fission. However, it was expected that

$$Q = \beta_1^2 - \left(\frac{\pi}{\tau+2\ell}\right)^2,$$

where β_1 is the first transport eigenvalue [2], would yield better results. By examining both the normal beam and the point source data for the two choices of Q, the most optimum choice is apparently given by equation (3.12). This choice forces the diffusion solution to decay in $\tilde{r}$ at the same rate as the transport solution (for large $\tilde{r}$) because the first modes dominate for $\tilde{r} >> 1$. The numerical data bears this out since the $Q = \beta_1^2 - \left(\frac{\pi}{\tau+2\ell}\right)^2$ solution is nearly identical to the transport solution for $\tau \gtrsim 3$. Unfortunately, this choice of Q does not consistently

improve the results near the source (or near the boundaries) since the assumptions for Fick's law are not valid in these regions and since the first mode does not dominate the solution for small $\tilde{r}$. A plot of β_1 vs τ is given in G. Garrettson's thesis for c = 0.9, and data for other c's is contained in an appendix [2].

A comparison of results in the τ = 10 and τ = 3 slabs (refs. Figs. 3-10), indicates that diffusion theory is more accurate in thick slabs. This is to be expected since Fick's law is not valid near the boundaries, and in a thin slab the neutron is never very far from one of the two boundaries.

D. CONCLUSIONS

In general, one can say that the neutron density computed using diffusion theory can be expected to yield reasonably accurate results except as indicated in the shaded areas of Fig. 17. If one is not interested in the density within about three m.f.p. from the source and within about one-half m.f.p. from the edges, diffusion theory can successfully be used. However, if one is interested in the density within these regions (e.g., the shaded areas in Fig. 17), it will be necessary to resort to the more rigorous and time-consuming techniques of transport theory to obtain accurate results.

One shouod also consider that the diffusion theory solution requires very long to compute for small radial distances from the source, since the smaller $|\tilde{\underline{r}}-\tilde{\underline{r}}'|$ is, the more terms the truncated series includes. For example, computer runs which included r = 0.01 required as long as 18.5 minutes to complete, which is comparable to the computation time required for the most difficult transport theory solutions. These runs, even

though lengthy, did not provide accurate data, and one must conclude that only the transport theory solution should be used to compute densities at very small radial distances.

Lastly, the choice of the parameter Q is an important factor in obtaining agreement between the results of diffusion theory and transport theory in the regions where the diffusion equation is valid. The choice (3.12) significantly decreases the discrepancy between the two results at large radial distances from the source, e.g., $\tilde{r} \gtrsim 3$ m.f.p.

In shielding problems with beam sources, the effect of these discrepancies will probably be most noted when calculating the transmission or reflection from the region of the beam. In these regions the diffusion results are most inaccurate since the emerging current from a region of the slab is a function of the neutron density in that region [3]. Diffusion theory should give satisfactory results for both transmission and reflection from regions not too near the beam.

E. SUGGESTIONS FOR POSSIBLE EXTENSIONS

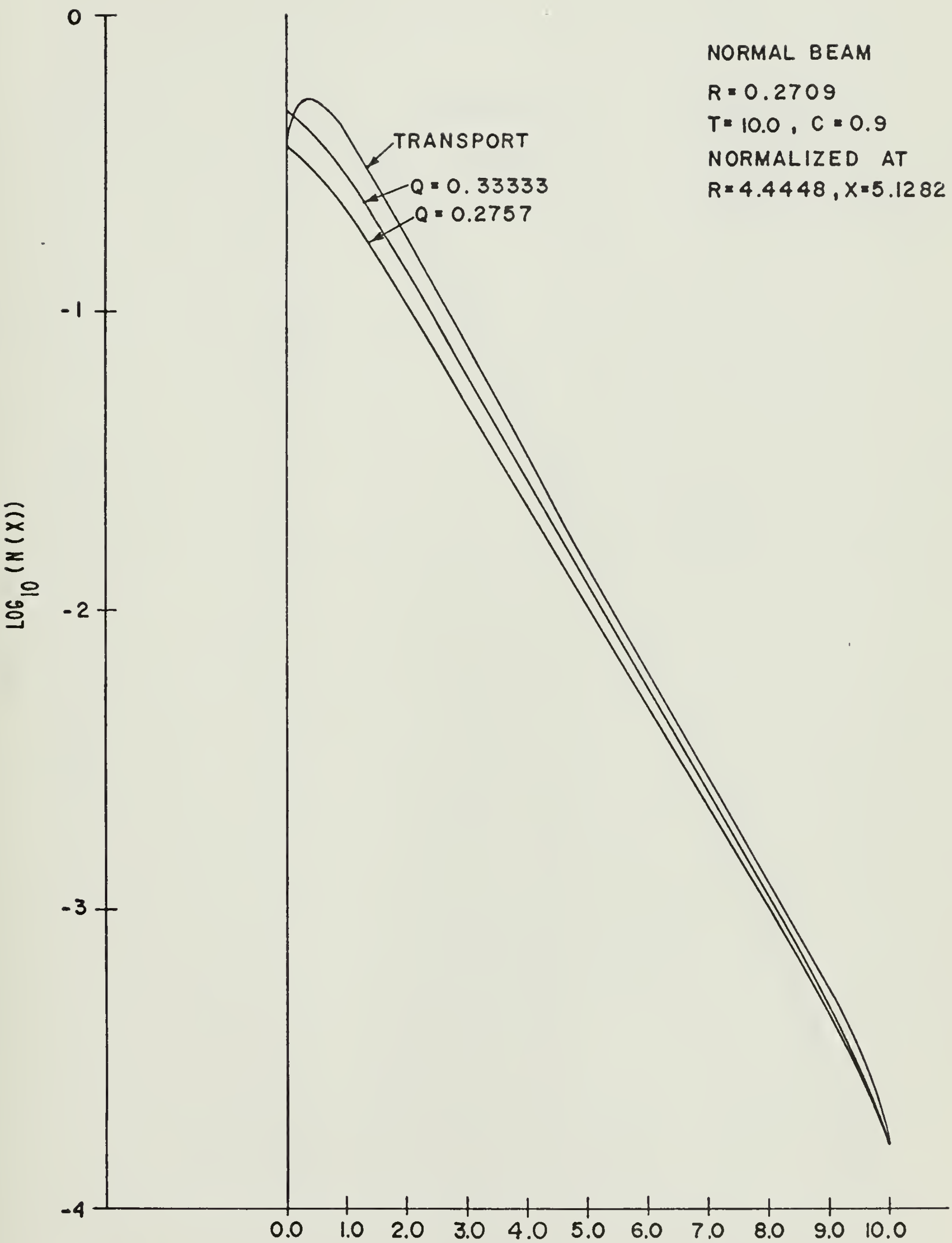
For slabs sufficiently thin, no discrete poles exist for the transport equation [2]. In these cases, to choose a proper value for Q, an effective mode of the transport equation would have to be found empirically. This could be done by making a semilog plot of the transport solution for fixed x, as a function of $\tilde{r}$ (for large $\tilde{r}$), and using the slope to determine the effective decay constant. Mathematically, this would correspond to the smallest "effective" pole in the continuous spectrum of the transport operator. These effective poles should be investigated, not only empirically, as mentioned above, but also mathematically.

Further, it would be interesting to investigate the results obtained over a wide range of values of both τ and c. One would expect diffusion theory to be less accurate for small τ, because of leakage, and also for small $c = \frac{\Sigma_s + \nu\Sigma_f}{\Sigma}$, which corresponds to a highly absorbing slab. The diffusion approximation is not expected to be valid unless $\Sigma_a << \Sigma_s$. (Ref. Chapter II).

APPENDIX 1 - Numerical Results

Appendix 1 contains graphical displays comparing numerical data obtained using transport theory with that obtained using diffusion theory. Figures 3-10 represent semi-log plots of the neutron density in a slab, as a function of normal depth, from a pencil beam normally incident to the slab, for various radial distances from the beam path. Figures 11-16 represent semi-log plots of the neutron density in a slab, as a function of normal depth, from a point source within the slab, for various radial distances from the source.

This data is discussed in Chapter IV.



SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 3

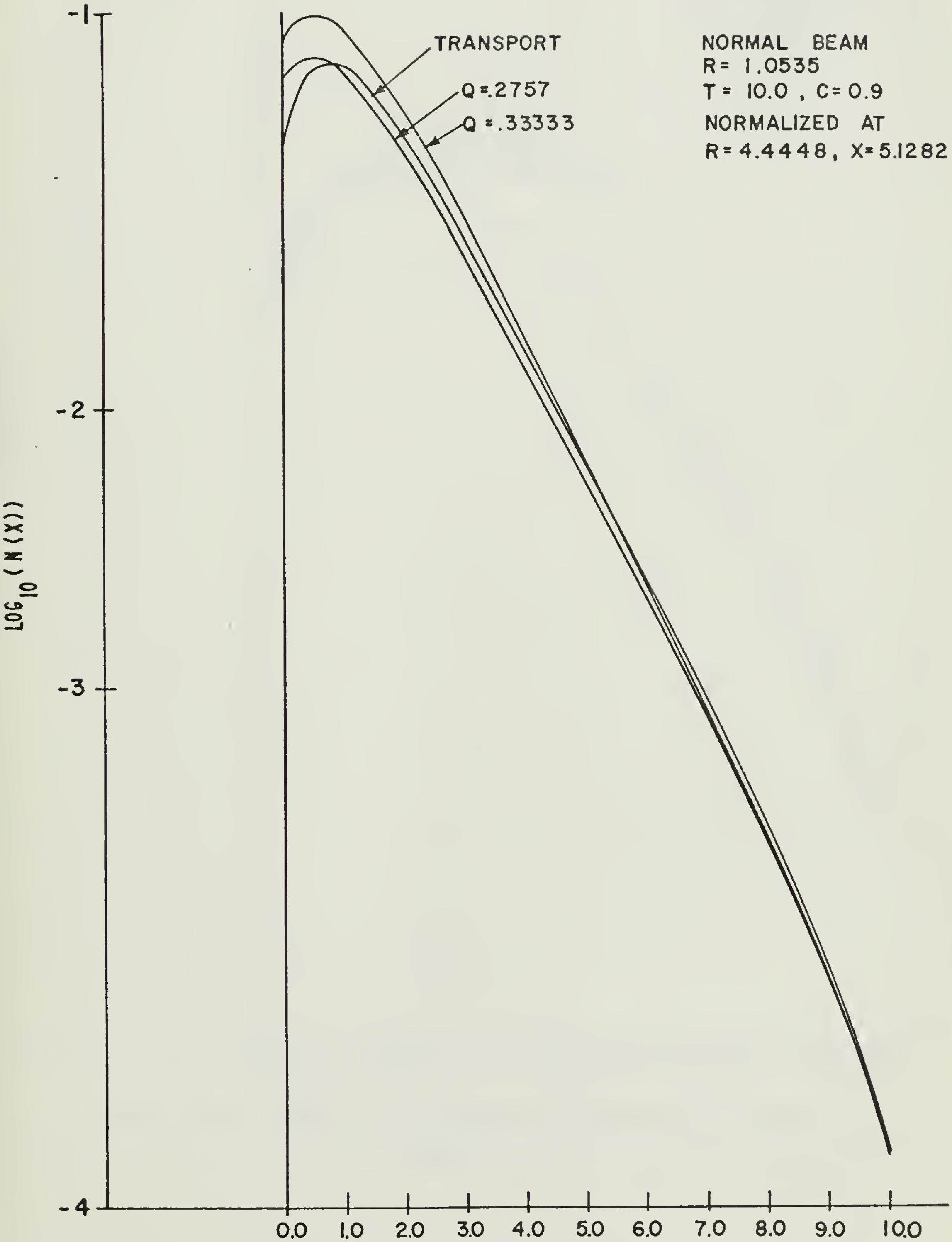
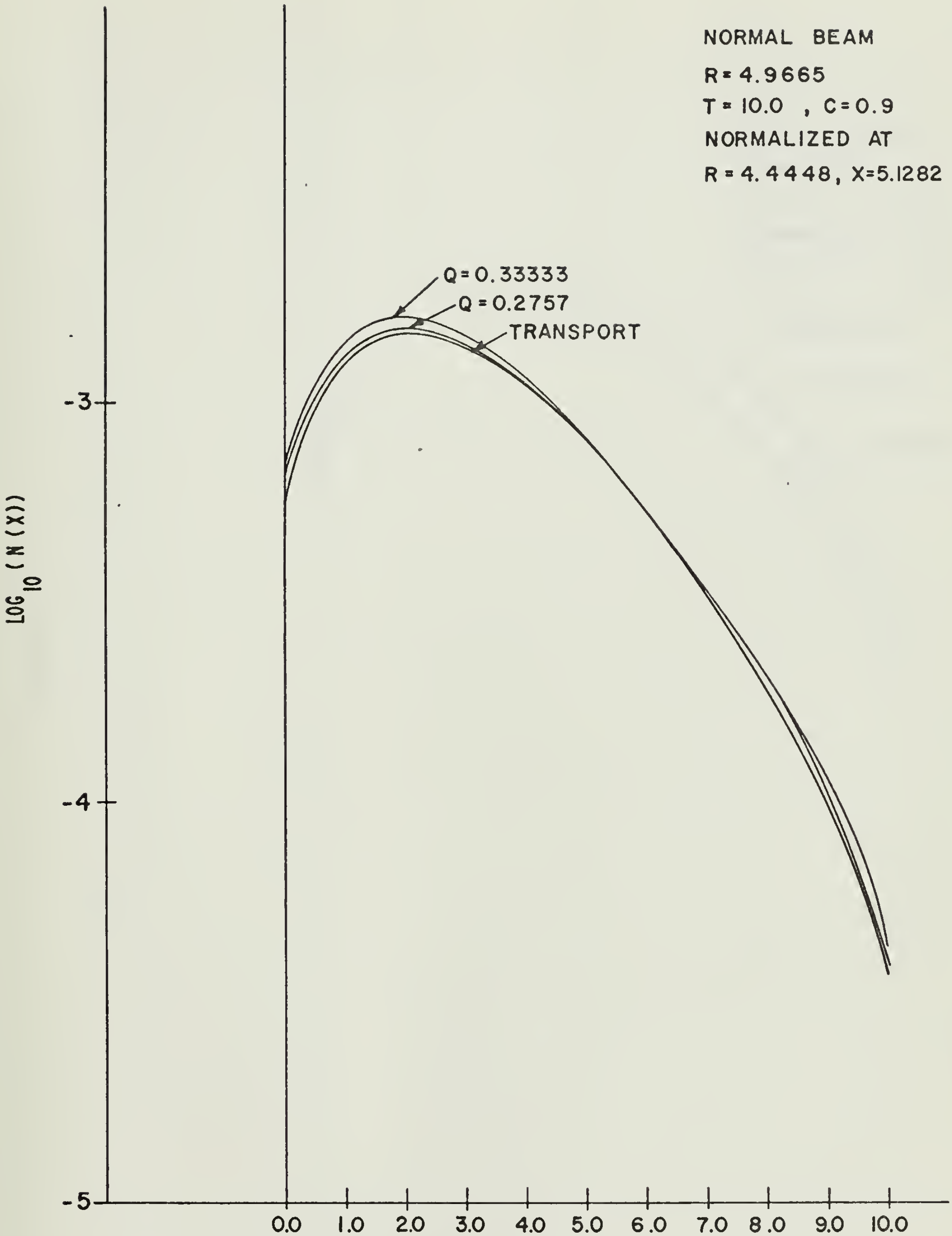
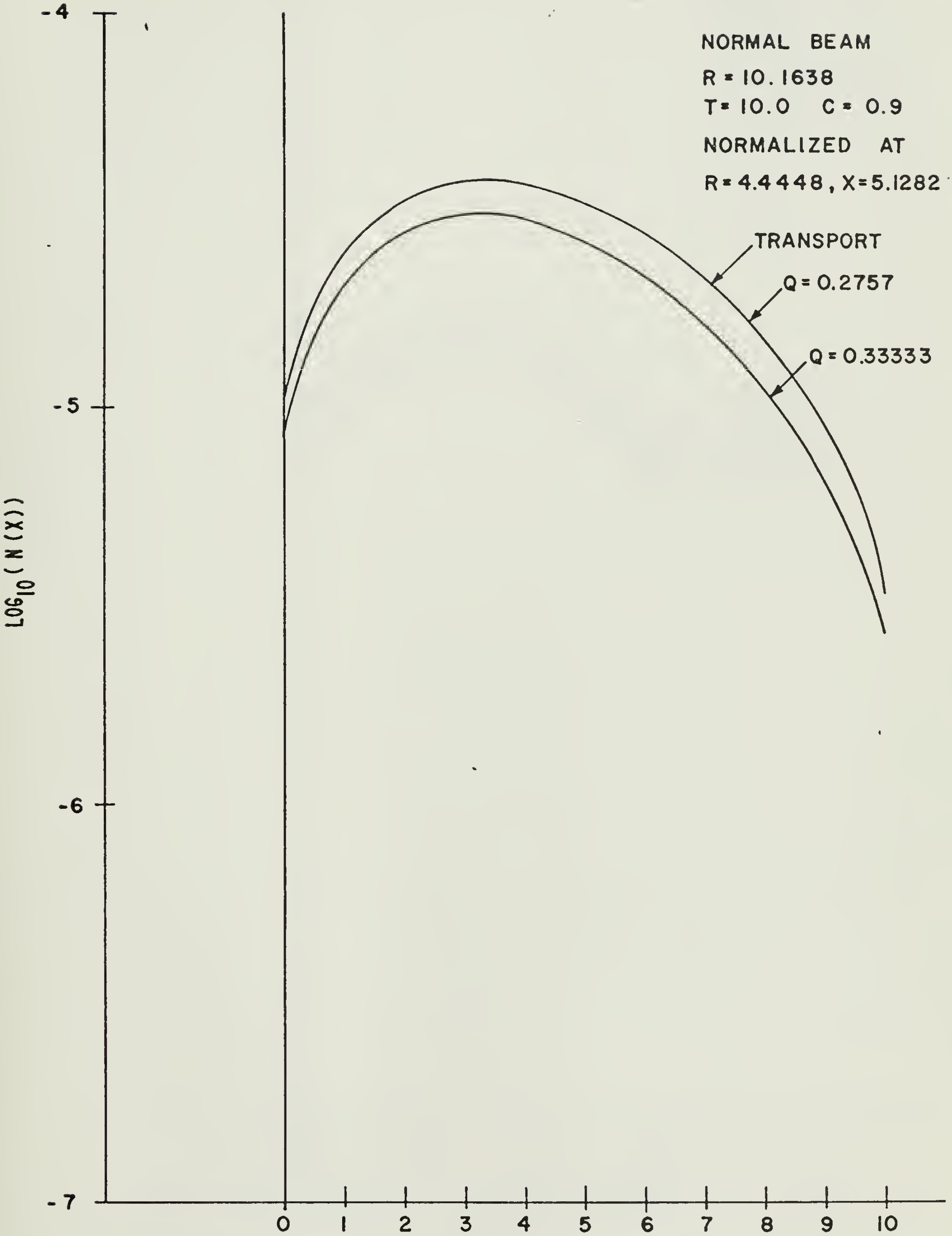


FIG. 4: SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB



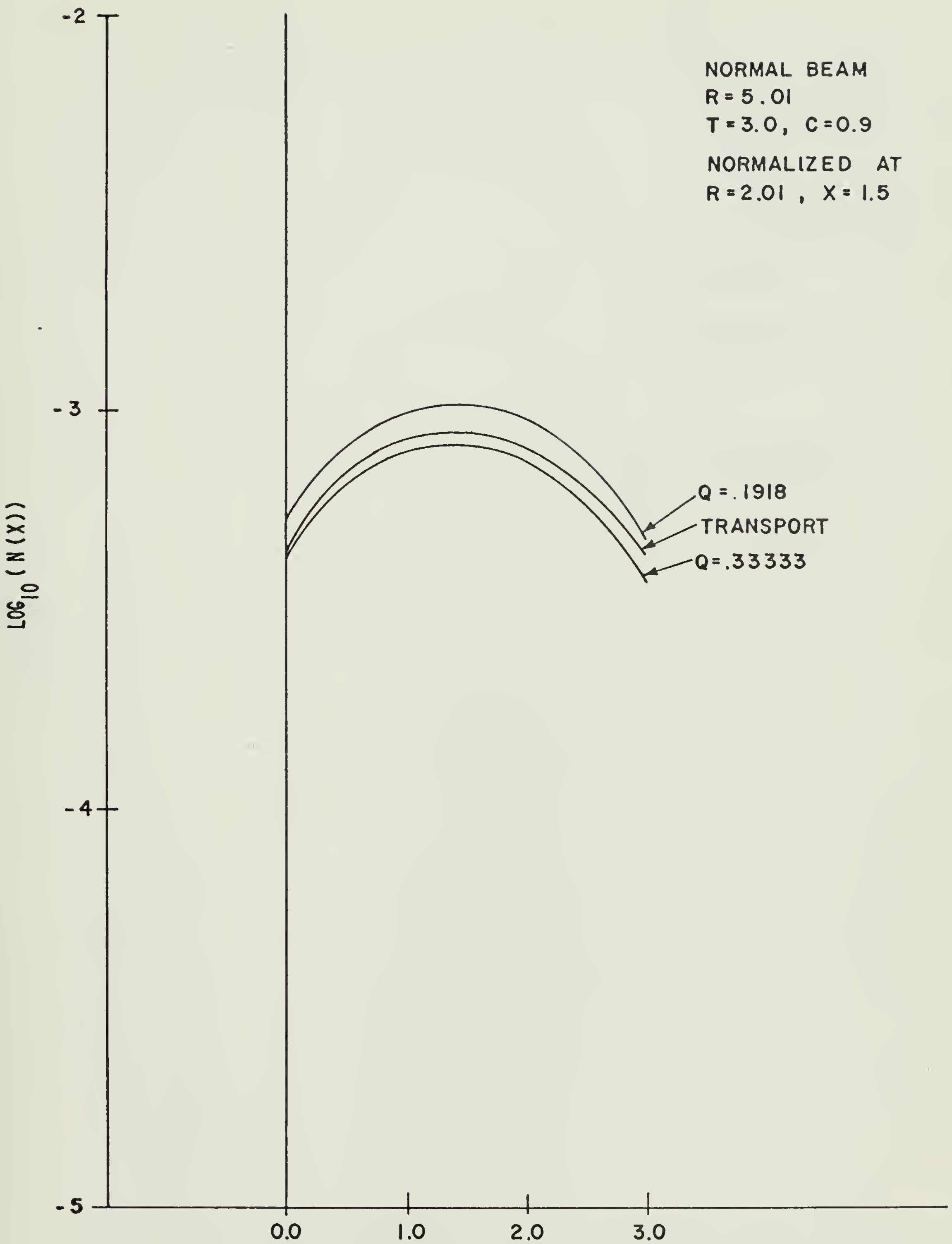
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 5



SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 6



SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 7

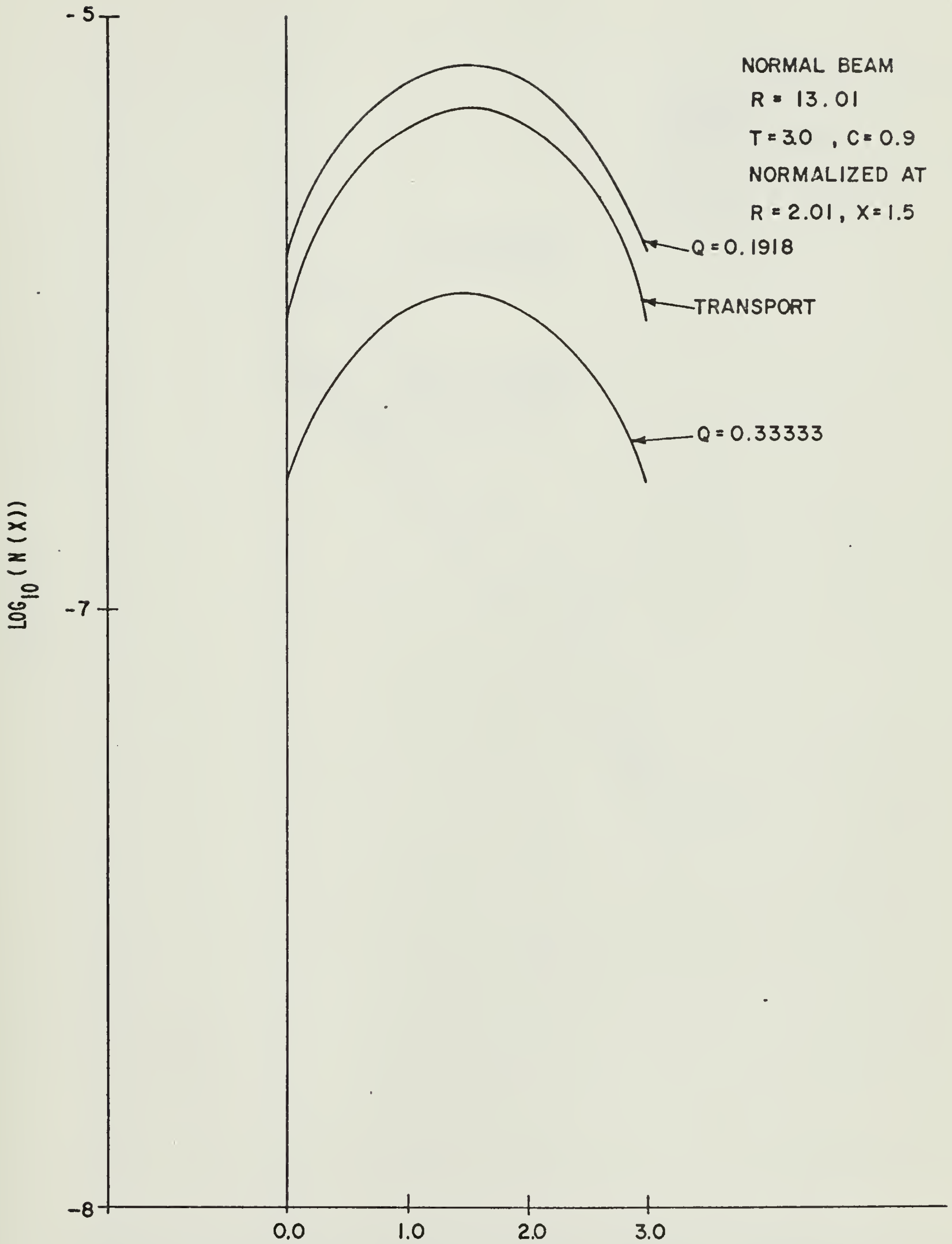
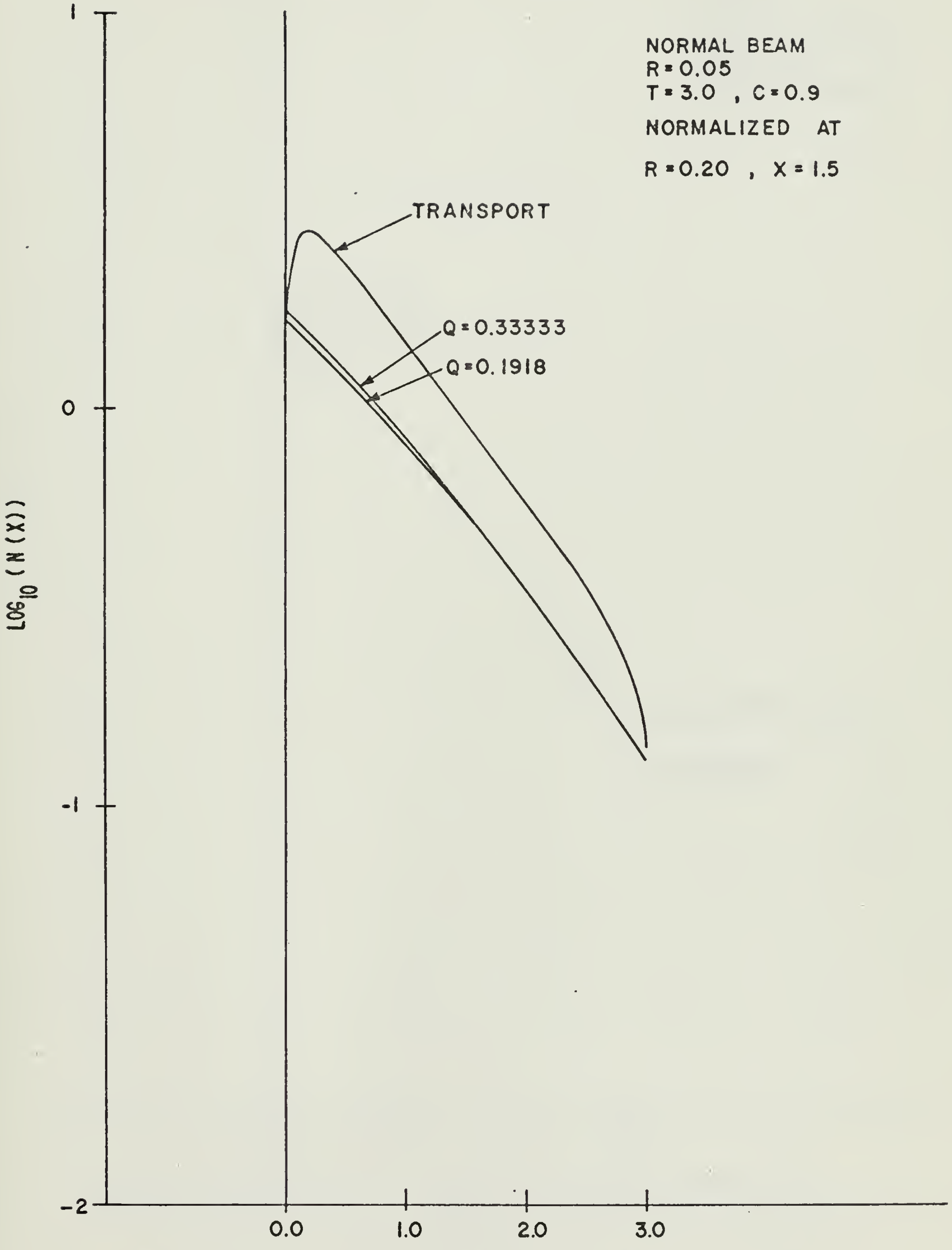
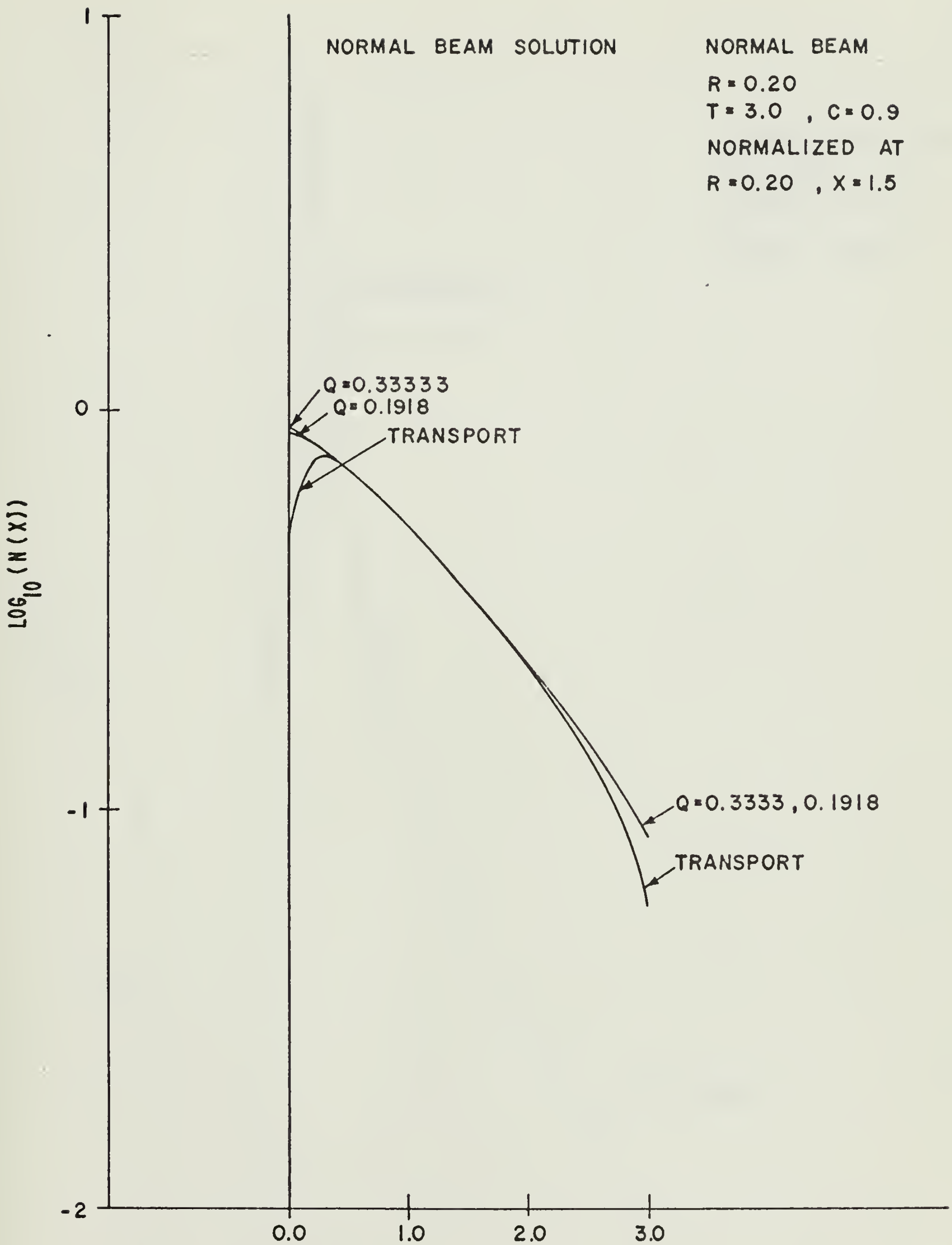


FIG. 8: SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB



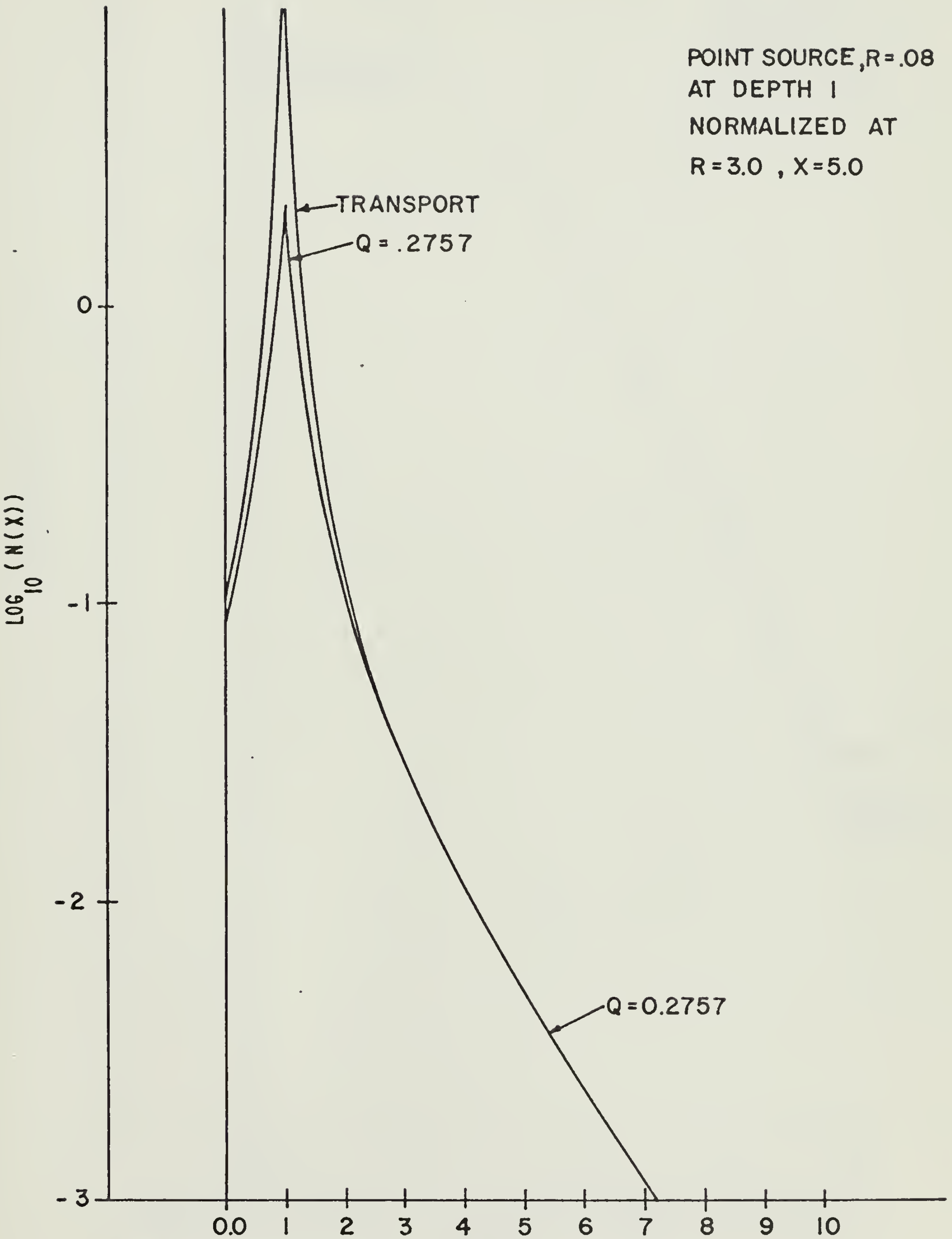
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 9



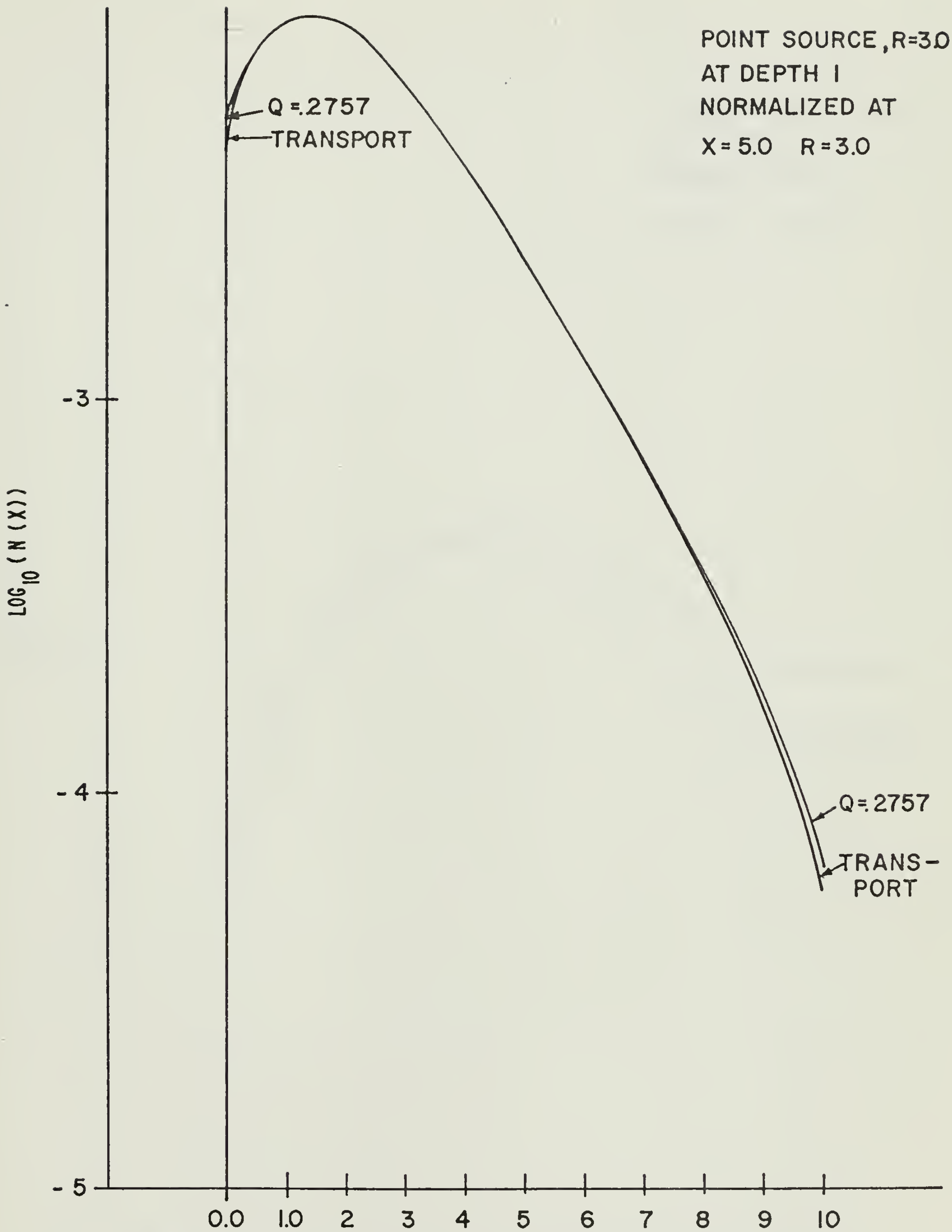
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 10



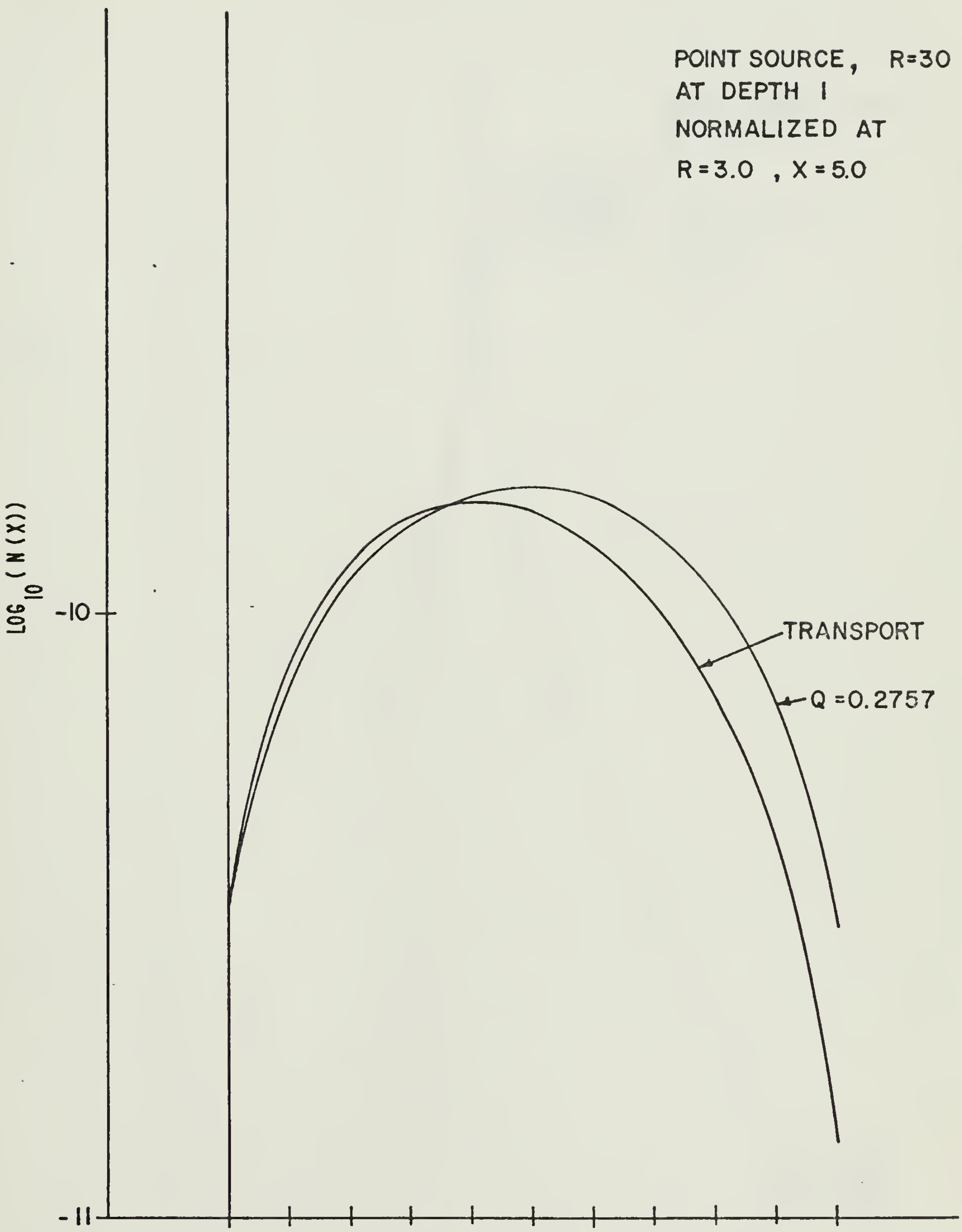
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 11



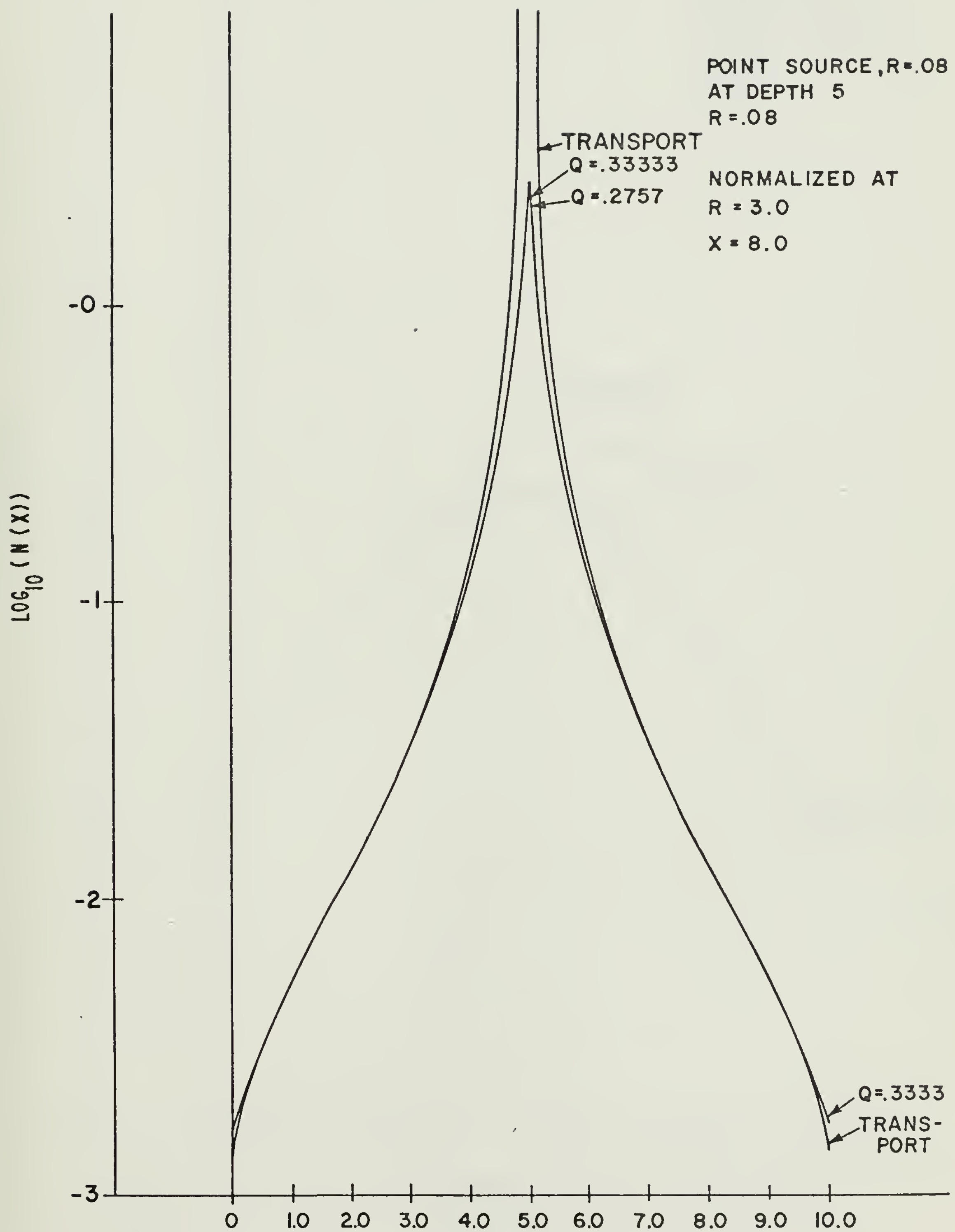
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 12



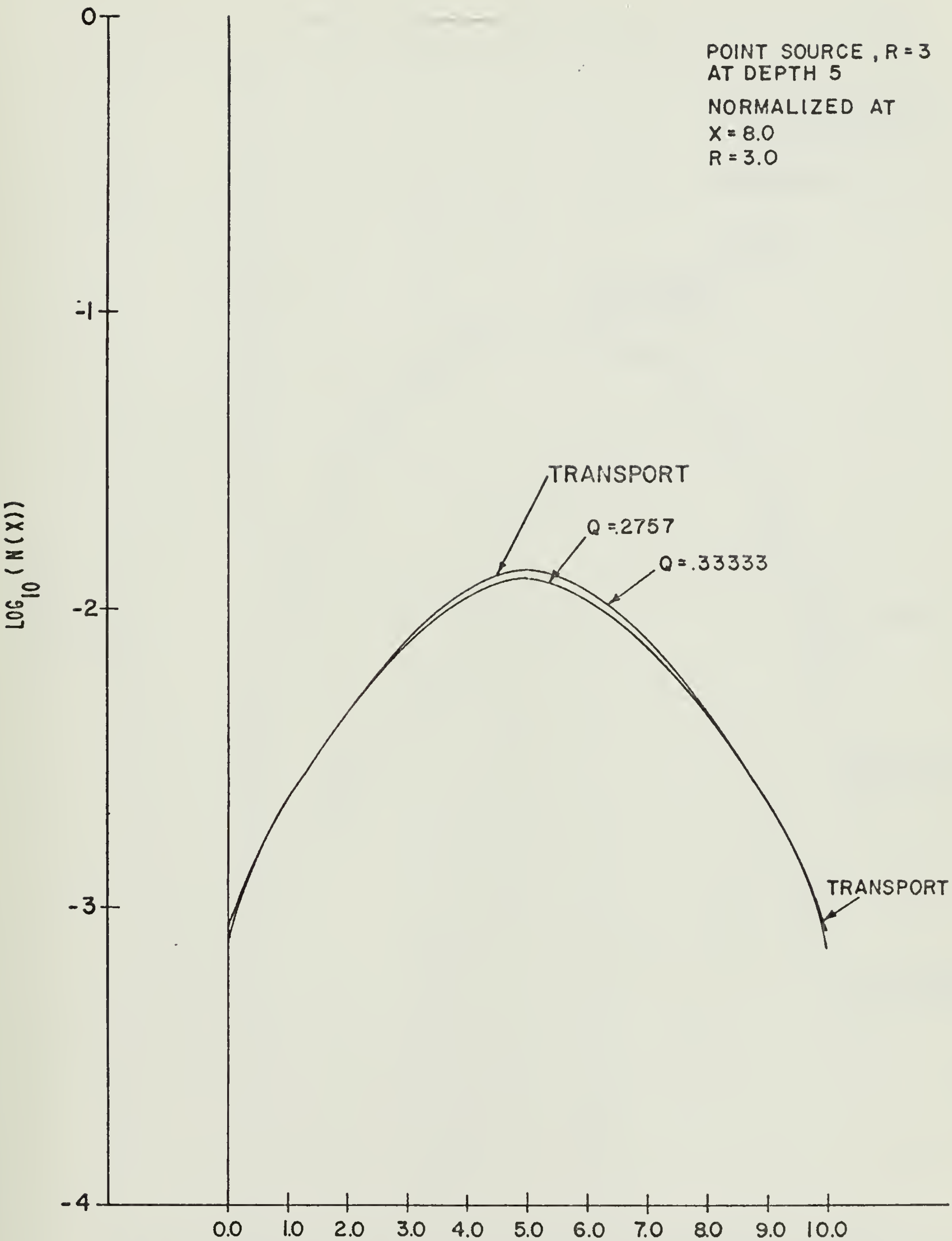
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 13



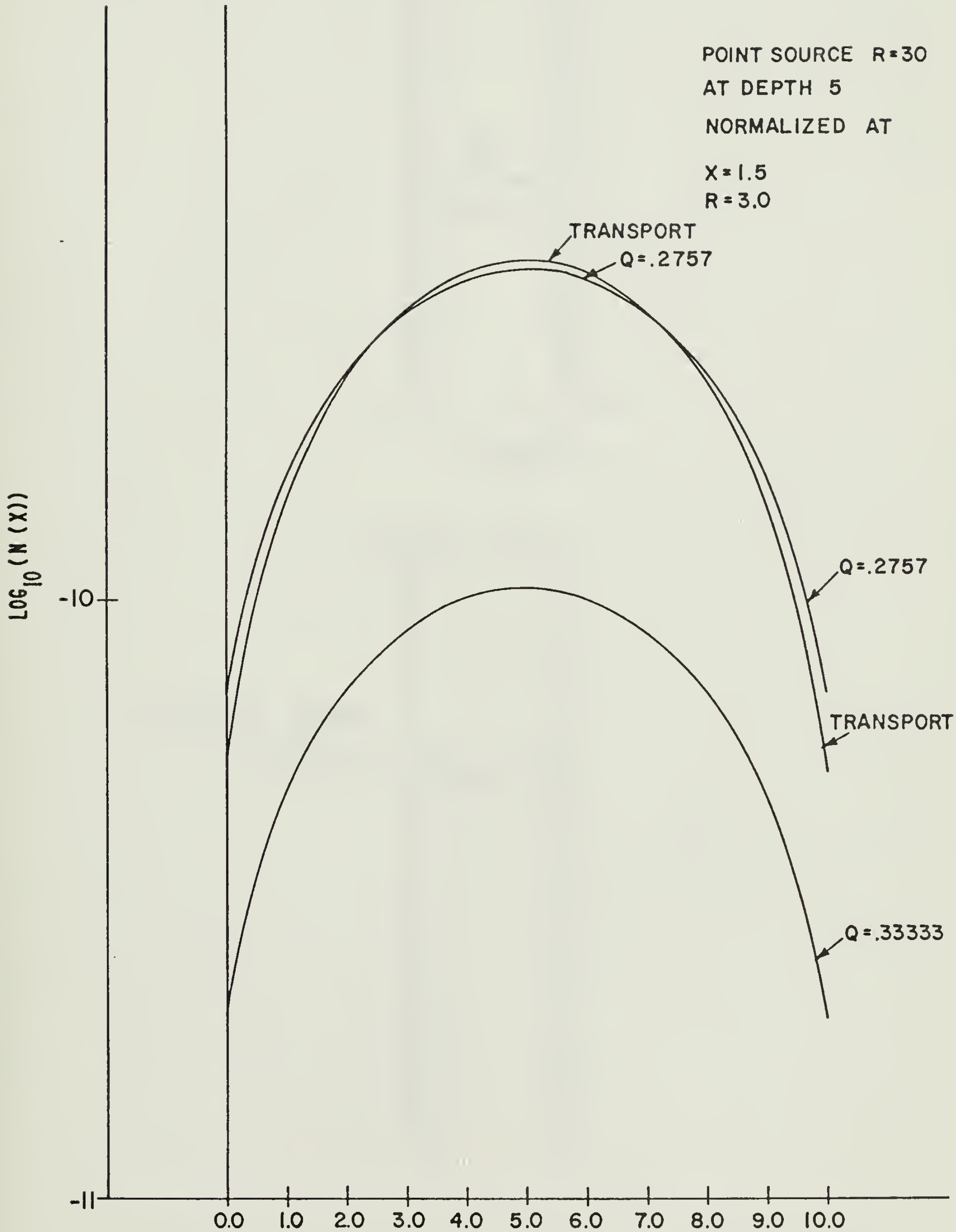
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG.14



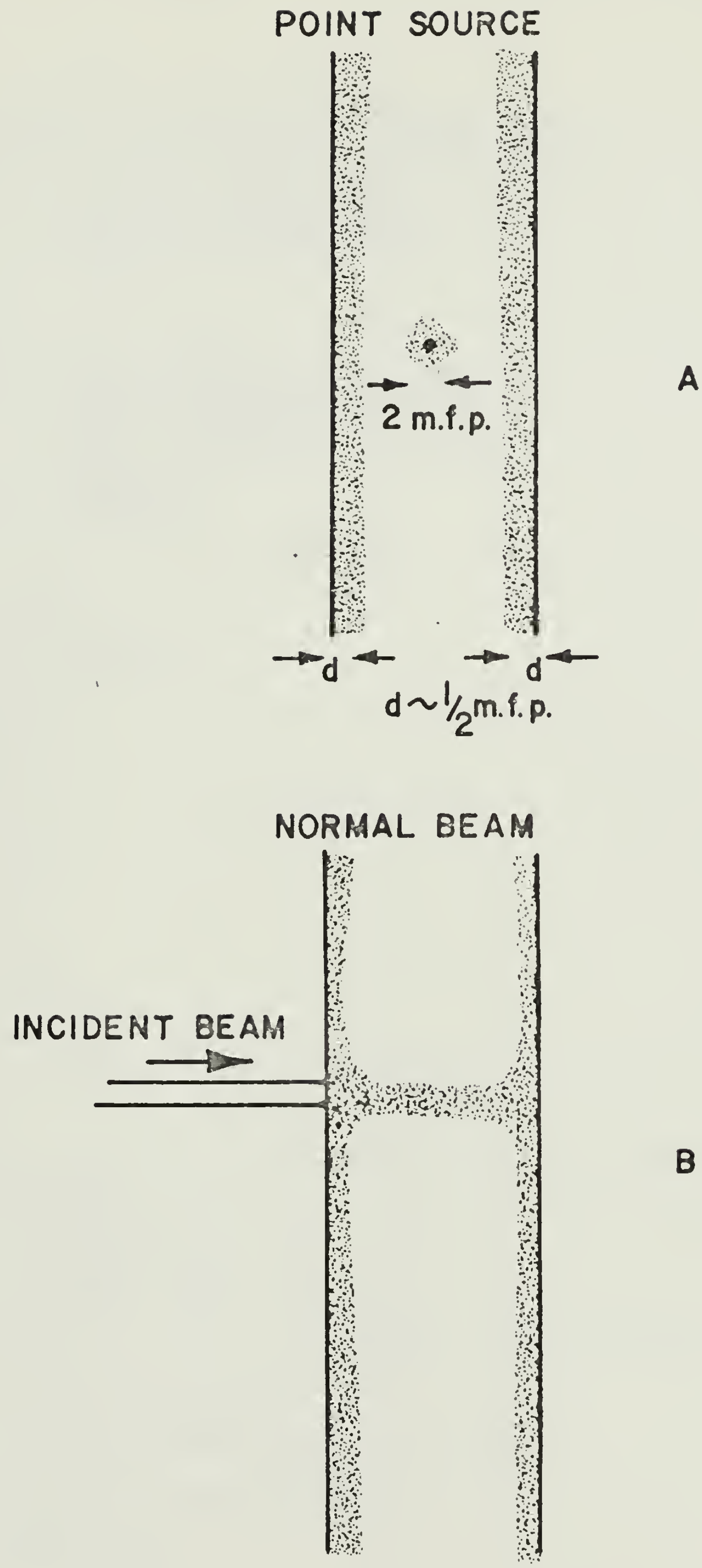
SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 15



SEMILOG PLOT OF DENSITY AS A FUNCTION OF DISTANCE IN THE SLAB

FIG. 16



REGIONS OF INACCURACY FOR DIFFUSION THEORY

FIG. 17

APPENDIX 2 - Fortran IV Program Listing

```
C   STUDY OF NEUTRCN DIFFUSION
C
      REAL*4 NUB  , NVAL, NUM, MODB
      DIMENSICN B(100,100) , PT(100,100)
      DIMENSION XMESH (100) , RMESH (100)
      READ(5,101)EPS,XPRI,TAU,C,D
      WRITE(6,101)EPS,XPRI,TAU,C,D
      READ(5,111)NVAL,PTVAL,R,Z,Y
      WRITE(6,111)NVAL,PTVAL,R,Z,Y
  111 FORMAT(5F10.6)
      NR=13
      NX=35
C THE 35 XMESH PTS ARE
      READ(5,1000)(RMESH(K),K=1,NR)
      WRITE(6,1000)(RMESH(K),K=1,NR)
      READ (5,121) (XMESH(J),J=1,NX)
      WRITE(6,121) (XMESH(J),J=1,NX)
  121 FORMAT (6F10.5)
  101 FORMAT(5F10.5)
 1000 FORMAT (5F10.5)
      M=0
      TEMP=0.0
      NUM=0.0
      MODB=0.0
      PI=3.141593
      T=TAU+(2.*EPS)
      AR=0.0
      DCY=0.0
      ALPMR=0.0
      FUD=0.0
      CH=0.0
      A=0.0
      XSYN=0.0
      BESL=0.0
      TO=0.0
      NUB=0.0
      CK=0.0
      C2=0.0
      Z=Z+EPS
      Y=Y + EPS
      XP=0.0
      XP=XPRI+EPS
C
C COMPUTE THE NORMALIZING CONSTANTS
    5 M=M+1
      AB=M
      DKY=AB*(1.-(((-1.)**M)*EXP(-T  )))/((AB*PI)**2+(T**2))
      C2=AB*PI/T
      A=R*SQRT(D+(C2**2))
      XSYN=SIN(C2*Z)
      CALL BESK(A,0,BK,IER)
      IF (IER.EQ.0) GO TO 200
      WRITE(6,201) IER
  201 FORMAT('0','***** THE BESSEL ERROR IS',I3,'*****')
  200 CONTINUE
      BESL=BK
      TO=TO+(DKY*XSYN*BESL)
      NUB=NUB +(2./T)*SIN(C2*Y)*XSYN*BESL
C COMPUTE SIZE OF BESSEL FN
      CK=BESL/TO
      IF(ABS(CK)-0.0005)125,5,5
  125 CONTINUE
      CCNN=NVAL/TO
      CCNP=PTVAL/NUB
      M=0
      DO 3 K=1,NR
      AR=RMESH(K)
      DO 4 J=1,NX
      X=XMESH(J)
      AX=X+EPS
  120 M=M+1
      AM=M
```

```
C
C
C   CCMPUTE DECAY TERM, DCY
C
        DCY=AM*(1.-(((-1.)**M)*EXP(-T)))/((AM*PI)**2+(T**2))
C
C   CCMPUTW FRACTICN M*PI/T=C1
        C1=AM*PI/T
C
C
C   COMPUTE ALPMR
        ALPMR=AR*SQRT((D)+(C1**2))
C
C   SIN X TERM
        FUD= SIN(C1*AX)
C
C   BESSEL FN TERM
        CALL BESK(ALPMR,0,BK,IER)
        IF (IER.EQ.0) GO TO 202
        WRITE(6,201) IER
  202   CCNTINUE
        MODB=BK
C
        TEMP=TEMP +(DCY*MODB*FUD)
C
C  CCMPUTE VALUE FROM POINT SOURCE
C
        NUM=NUM+((2./T)*SIN(C1*XP)*FUD*MODB)
C  CHECK VALUE OF BESSEL FN
C
        CH=MODB/TEMP
        IF (ABS(CH)-0.0005)14C,120,120
  140   CCNTINUE
        B(J,K)=CONN*TEMP
        PT(J,K)=CONP*NUM
        M=0
        NUM=0.0
        TEMP=0.00
    4   CONTINUE
    3   CONTINUE
  500   FORMAT('0','TAU = ',F9.6,'    ,C =   ',F9.6,'    ,AND D =
        WRITE(6,500) TAU,C,D
  501   FORMAT(//'0','THE',I3,' X MESH POINTS ARE'/)
  502   FORMAT('0',10F12.6)
        WRITE(6,501) NX
        WRITE (6,502)(XMESH(J),J=1,NX)
  503   FORMAT('1')
        WRITE(6,503)
  504   FCRMAT ('0','PT SOURCE AT DEPTH',F9.6/'0',' DENSITIES
        WRITE(6,504)XPRI
  505   FCRMAT('0','R =',F8.4,4X,1P10E11.3/('0',15X,1P10E11.3)
        DO 105 K=1,NR
        WRITE(6,505) RMESH(K),(PT(J,K),J=1,NX)
        WRITE(6,507)
  508   FORMAT (30('*'),'R =', F8.4,'  FOLLOWS',30('*'))
  105   CONTINUE
        WRITE(6,503)
  506   FORMAT('0','THE NORMAL BEAM DENSITIES ARE'//)
        WRITE (6,506)
        DO 106 K=1,NR
        WRITE(6,505) RMESH(K) , (B(J,K),J=1,NX)
        WRITE (6,507)
  507   FCRMAT ('0')
        WRITE(7,508) RMESH (K)
  509   FORMAT(1P8E10.3)
        WRITE (7,509) (B(J,K), J=1,NX)
  106   CCNTINUE
        STOP
        END
```

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UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Naval Postgraduate School Monterey, California 93940	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b. GROUP

3. REPORT TITLE

Neutron Transport from a Point Source in a Slab; A Comparison Between Diffusion Theory and Transport Theory

4. DESCRIPTIVE NOTES (Type of report and, inclusive dates)

Master's Thesis, September 1970

5. AUTHOR(S) (First name, middle initial, last name)

John H. Shimerda

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
September 1970	52	9

8a. CONTRACT OR GRANT NO. N/A b. PROJECT NO. N/A c. N/A d.	9a. ORIGINATOR'S REPORT NUMBER(S) N/A 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) N/A

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11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
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13. ABSTRACT

The one-speed, steady state, diffusion equation was solved for a point source and for a normal pencil beam in a homogeneous, isotropically scattering slab. Numerical results obtained using diffusion theory were compared to available transport theory results for two slab thicknesses.

This comparison demonstrated that the diffusion theory approximation to the transport equation will yield accurate results except within about one-half mean free path of a boundary and except within about three mean free paths of a source. The best agreement between diffusion theory and transport theory is obtained if the first radial buckling constant in the diffusion solution is chosen equal to the radial buckling computed using transport theory.

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S/N 0101-807-6811

UNCLASSIFIED

Security Classification

A-31408

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Neutron						
Radiation						
Diffusion Theory						
Transport Theory						
Boltzmann Equation						
Green's Functions						
Shielding						

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